Auxiliary potential in no-core shell-model calculations

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Abstract

The Lee-Suzuki iteration method is used to include the folded diagrams in the calculation of the two-body effective interaction $v_{\text{eff}}^{(2)}$ between two nucleons in a no-core model space. This effective interaction still depends upon the choice of single-particle basis utilized in the shell-model calculation. Using a harmonic-oscillator single-particle basis and the Reid-soft-core NN potential, we find that $v_{\text{eff}}^{(2)}$ overbinds ^{4}He in 0, 2, and $4\hbar\Omega$ model spaces. As the size of the model space increases, the amount of overbinding decreases significantly. This problem of overbinding in small model spaces is due to neglecting effective three- and four-body forces. Contributions of effective many-body forces are suppressed by using the Brueckner-Hartree-Fock single-particle Hamiltonian.

1   Introduction

Previous calculations of the shell-model effective interaction involved a number of uncertainties. The major ones included the choice of the single-particle (s.p.) basis, the choice of the starting energy ω in the Brueckner G-matrix [1] calculation, the neglected contribution from higher-order core-polarization diagrams, and the effects of both the real and effective three- and higher-body forces. It was proposed in Ref.[2] that the core-polarization diagrams could be eliminated by adopting a no-core model space, in which all the nucleons in a nucleus are treated as active. In Refs.[3, 4], the no-core approach has been used and satisfactory results are obtained for light nuclei.

The results of this no-core approach depend on the choice of the starting energy for the G-matrix. One may argue that this uncertainty in the choice of the starting energy ω can be avoided by evaluating an energy-independent interaction employing the iteration methods proposed by Lee and Suzuki [5] and Krenciglowa and Kuo [6]. Applying this technique, one can sum the folded diagrams to all orders to obtain a starting-energy-independent effective interaction $v_{\text{eff}}^{(2)}$. Therefore, with the use of a no-core space and including the folded diagrams, the effective interaction obtained is subject to only two of the major uncertainties mentioned above, i.e., the choice of the s.p. basis and the effect of the neglected effective three- and higher-body forces.

These two remaining uncertainties are related. With an optimally chosen s.p. basis, the contribution from the effective many-body forces could be minimized [7]. Furthermore, both of the uncertainties are related to the size of the model space and are expected to diminish as the size increases. Indeed, the effective interaction is only introduced with the truncation of the infinite Hilbert space to a finite-size model space. Furthermore, one should keep in mind that so-called Q-box diagrams, like the one displayed in Fig. 1a, are not the only source of effective many-body forces. Even if the Q-box is restricted to two-body terms, which means the G-matrix for no-core calculations, the inclusion of folded diagrams yields effective three-body forces (see

Fig. 1b). It has been demonstrated that such many-body forces are non-negligible [8], in particular if a large number of active particles has to be considered [9]. As we will discuss below, one may try to minimize the effects of such many-body forces by introducing an appropriate auxiliary field. One may view the present effort as an extension of the work of Ref.[7] to the case of realistic NN potentials which capitalizes on the results presented in Refs.[8, 9].

In this work, we will use the Lee-Suzuki method [5] to calculate the starting-energy-independent two-body effective interactions $v_{\text{eff}}^{(2)}$ for no-core, harmonic-oscillator (HO) model spaces and study the dependence of the shell-model results obtained for ^{4}He with $v_{\text{eff}}^{(2)}$ on the HO basis parameter $\hbar\Omega$ and the size of the model space. It has been noticed in a previous work [10] that $v_{\text{eff}}^{(2)}$ tends to overbind light nuclei. Here we will show that the overbinding is quite significant when the model space is relatively small. We will show that the overbinding problem can be cured by introducing an auxiliary field, such as the Brueckner-Hartree-Fock (BHF) approximation.

After this introduction we will present some details on the evaluation of the energy-independent effective two-body force for no-core shell-model calculations in section 2. Numerical results for the binding energy of ^{4}He will be presented in section 3. In section 4 we will discuss the influence of an auxiliary potential, and section 5 contains the conclusions of the present investigation.

2   Calculation of $v_{\text{eff}}^{(2)}$

The Brueckner G matrix is calculated according to the following equation:

$$G(\omega) = v_{12} + v_{12}\frac{Q}{\omega - (h_1 + h_2 + v_{12})}v_{12}, \tag{1}$$

where v_{12} is the NN force for which we will use the Reid-soft-core (RSC) potential [11], ω is the starting energy, Q is the Pauli operator which excludes the scattering into the two-particle states inside the model space. For a full no-core $N\hbar\Omega$ space, we

define Q as

$$
\begin{aligned}
Q &= 0 \quad \text{for} \ \ n_1 + n_2 \leq N \\
  &= 1 \quad \text{for} \ \ n_1 + n_2 > N.
\end{aligned}
\tag{2}
$$

where $n_i = 2n_r(i) + l(i) = 0, 1, \ldots$, are the principal quantum numbers of the s.p. states occupied by the two intermediate-state nucleons in the multiple scattering process.

For the first part of our discussion (see section 4 for an alternative choice) the s.p. Hamiltonian in Eq.(1) is taken as

$$
h_i = t_i + u_i = \frac{\boldsymbol{p}_i^2}{2m} + (\frac{1}{2}m\Omega^2 r_i^2 - V_0) = t_i + (u_i^{\text{HO}} - V_0) = h_i^{\text{HO}} - V_0,
\tag{3}
$$

where we use a s.p. potential (u_i) that is of the shape of a harmonic oscillator but is shifted downward by an amount V_0 to make it more realistic. The quantity V_0 represents the depth of the mean field of the nuclear medium. It is convenient to define a shifted starting energy as $\omega' = (\omega + 2V_0)$ and rewrite Eq.(1) as

$$
G(\omega') = v_{12} + v_{12} \frac{Q}{\omega' - (h_1^{\text{HO}} + h_2^{\text{HO}} + v_{12})} v_{12},
\tag{4}
$$

where $h^{\text{HO}} = t_i + u_i^{\text{HO}}$ is now a pure HO Hamiltonian. Since we will use the Lee-Suzuki iteration method [5] to take into account the folded diagrams, the resulting effective interaction will be independent of the starting energy ω' as well as the shift V_0. Therefore, no specific choice for the value of V_0 needs to be made.

However, in the case when the folded diagrams were ignored (which is a common practice in effective-interaction calculations), one would have to choose a reasonable starting energy to minimize the contribution from the folded diagrams. It should then be noted that the starting energy ω' used in Eq.(4), unlike ω, does not correspond to the energy E_2 of the initial two-particle state in the ladder diagrams. Rather, it is related to $(E_2 + 2V_0)$. When the two nucleons in the initial state occupy bound s.p. states, E_2 is negative. But $\omega' \simeq (E_2 + 2V_0)$ could very well be positive. In fact,

it has been found [12, 13] that for the two valence neutrons in ^{18}O, a value of about 70 MeV for ω' yielded reasonable G-matrix elements.

In order to obtain the starting-energy-independent two-body effective interaction $v_{\text{eff}}^{(2)}$, we calculate $G(\omega')$ of Eq.(4) for 11 values of ω' ranging from about $-5\hbar\Omega$ to about $5\hbar\Omega$. These 11 sets of G matrices are then used to numerically calculate the derivatives of $G(\omega')$ with respect to ω' to the 9th order. Once the derivatives of $G(\omega')$ are obtained, we proceed with the Lee-Suzuki method to obtain $v_{\text{eff}}^{(2)}$. Here we point out that the number of iterations needed for convergence strongly depends on the value of ω' at which the derivatives are evaluated. It generally exceeds the number of derivatives retained in the iteration procedure.

In Fig.2, we show the values of the diagonal two-body matrix elements (TBMEs) of $G(\omega')$ and $v_{\text{eff}}^{(2)}$ in the states $|(0s_{1/2})^2\rangle_{J,T}$ with J=0, T=1 and J=1, T=0 for a wide range of ω'. For these matrix elements we use $\hbar\Omega$=16 MeV and the Pauli operator is defined in Eq.(2) with N=4. It can be seen from the figure that the matrix elements of $G(\omega')$ decrease (i.e., become more attractive) with increasing ω', while those of $v_{\text{eff}}^{(2)}$ are independent of ω'.

We also note in Fig.2 that there is a particular value of ω' for which the matrix elements of $G(\omega')$ are about equal to those of $v_{\text{eff}}^{(2)}$. This observation is the basis of an approximation scheme presented and tested in Ref.[10] and then used in Ref.[4].

3 Shell-Model Results

We perform the matrix diagonalization for the shell-model Hamiltonian

$$H_{\text{SM}} = \left(\sum_{i=1}^{A} t_i - T_{\text{c.m.}}\right) + \sum_{i<j}^{A} v_{\text{eff}}^{(2)}(ij) + V_{\text{Coulomb}} + \lambda(H_{\text{c.m.}} - \frac{3}{2}\hbar\Omega). \qquad (5)$$

In the above equation the $t_i = \mathbf{p}_i^2/(2m)$ are the one-body kinetic energies, $T_{\text{c.m.}} = (\sum_i \mathbf{p}_i)^2/(2mA)$ is the c.m. kinetic energy and V_{Coulomb} is the Coulomb interaction. The proton and neutron masses are taken to be the same. The last term (with λ=10)

in the above equation forces the c.m. motion of the low-lying states in the calculated spectrum to be in its lowest HO configuration.

In Fig.3, we plot the calculated ground-state (g.s.) energy of ^{4}He as a function of the HO basis parameter $\hbar\Omega$ for three model spaces of different sizes, $0\hbar\Omega$ ("$N=0$" curve), $2\hbar\Omega$ ("$N=2$" curve), and $4\hbar\Omega$ ("$N=4$" curve). In the $0\hbar\Omega$ model space which consists of only the $0s_{1/2}$ major shell, the g.s. energy begins at -33.9 MeV for $\hbar\Omega=10$ MeV, decreases to a minimum of -43.3 MeV at $\hbar\Omega=22$ MeV and then increases to -41.6 MeV for $\hbar\Omega=28$ MeV. These results significantly overbind the g.s. of ^{4}He. They are 5.6 to 15.0 MeV lower than the experimental g.s. energy of -28.3 MeV and are 9.3 to 18.7 MeV lower than the value of -24.6 MeV obtained in the (nearly exact) Green's function Monte Carlo (GFMC) approach [14] using the RSC potential.

In this one-major-shell model space, there is a simple way to obtain the above results. The g.s. energy of ^{4}He can be expressed in terms of the effective-interaction TBMEs as ($0s \equiv 0s_{1/2}$)

$$E_{\rm gs} = 3\left(\frac{3}{4}\hbar\Omega\right) + 3\left[\langle 0s^2|v_{\rm eff}^{(2)}|0s^2\rangle_{J=0,T=1} + \langle 0s^2|v_{\rm eff}^{(2)}|0s^2\rangle_{J=1,T=0}\right], \qquad (6)$$

where the first term is the kinetic energy (with the c.m. contribution subtracted) and the second term is the effective-interaction energy. According to Ref.[15], we know that for this one-dimensional model space, the effective-interaction TBMEs are related to the eigenenergies of the Schrödinger equation:

$$(h_1 + h_2 + v_{12})\phi_{J,T} = E_{J,T}\,\phi_{J,T} \qquad (7)$$

through

$$\langle 0s^2|v_{\rm eff}^{(2)}|0s^2\rangle_{J,T} = E_{J,T} - 2\left(\frac{3}{2}\hbar\Omega\right), \qquad (8)$$

where $\frac{3}{2}\hbar\Omega$ is the eigenenergy of the s.p. Hamiltonians h_1 and h_2 for the $0s_{1/2}$ state. For $\hbar\Omega=22$ MeV, we obtained

$$E_{0,1} = 55.183\,{\rm MeV} \quad \text{and} \quad E_{1,0} = 45.892\,{\rm MeV},$$

which lead to

$$\langle 0s^2|v_{\text{eff}}^{(2)}|0s^2\rangle_{0,1} = -10.817\,\text{MeV}$$

and

$$\langle 0s^2|v_{\text{eff}}^{(2)}|0s^2\rangle_{1,0} = -20.108\,\text{MeV}.$$

Therefore,

$$E_{\text{gs}} = 3\left(\frac{3}{4}\times 22\right) + 3(-10.817 - 20.108) = -43.275\,\text{MeV},$$

which agrees with the result that we obtained through the Lee-Suzuki iteration procedure. We further remark that the effective-interaction TBMEs $\langle 0s^2|v_{\text{eff}}^{(2)}|0s^2\rangle_{J,T}$ are equal to $G_{J,T}(\omega')$ with $\omega' = E_{J,T}$. This is another property observed in Ref.[15] for the effective interaction in a one-dimensional model space. From these arguments we can see that the overbinding in this very limited model space is related to the fact that the matrix elements $G_{J,T}(\omega' = E_{JT})$ are very attractive for the rather positive values of $E_{0,1}$ and $E_{1,0}$.

Note that in the limit of $\hbar\Omega = 0$, the one-dimensional model-space result for the g.s. energy of ^{4}He is

$$E_{\text{gs}} = 3(0 - 2.2246) = -6.6738\,\text{MeV} \quad (\text{for } \hbar\Omega = 0), \tag{9}$$

where -2.2246 MeV and 0 are the lowest eigenenergies of the two-body system with J=1, T=0 (deuteron) and J=0, T=1, respectively. This (-6.6738 MeV) is the limit that the "N=0" curve in Fig.2 will approach as $\hbar\Omega \to 0$.

In the $2\hbar\Omega$ model space, the results for the binding energy of ^{4}He are reduced considerably (see Fig.3) although they are still larger than the experimental value as well as the more exact theoretical value for the RSC potential. Note that the value of $\hbar\Omega$ at which the lowest g.s. energy is obtained is between 16 MeV and 18 MeV in the $2\hbar\Omega$ model space (N=2). This is quite different from corresponding value of $\hbar\Omega$=22 MeV with the $0\hbar\Omega$ space (N=0). At $\hbar\Omega$=16 MeV, the $2\hbar\Omega$ result for the binding

energy is 33.6 MeV, which still overbinds the g.s. by a large amount. The reduction of the calculated energy with increasing model space can easily be understood from the following observations: If the model space is increased, the Pauli operator Q in the Bethe-Goldstone Eq.(1) ensures that the energy ω_1 of the lowest pole in G is shifted to higher energies, as this energy correspond to the energy of the lowest 2 particle state outside the model space. Therefore the matrix elements of G calculated at the same starting energy are less attractive for the larger model space. The net effect of enlarging the model space with the appropriately recalculated effective interaction at the two-particle level is to reduce the overbinding.

The results continue to improve as we increase the model space from $2\hbar\Omega$ to $4\hbar\Omega$. Now the lowest g.s. energy of about -31.9 MeV is found when $\hbar\Omega$ falls between 14 and 16 MeV. This lowest energy is about 1.7 and 11.4 MeV higher than the corresponding values of -33.6 MeV and -43.3 MeV for the $2\hbar\Omega$ and $0\hbar\Omega$ spaces, respectively.

The dependence of the results on the $\hbar\Omega$ value also weakens substantially as we go from $2\hbar\Omega$ to $2\hbar\Omega$ and to $4\hbar\Omega$. We can quantify this dependence by defining a dimensionless parameter

$$C_a \equiv \text{Average of} \quad \frac{|E_{\text{gs}}(\hbar\Omega + 2) - E_{\text{gs}}(\Omega)|}{2\text{MeV}} \tag{10}$$

that characterizes the "average curvature". For the $N=0$ curve in Fig.3, C_a is 0.61. It decreases to 0.39 for the $N=2$ curve; and it further reduces to 0.27 for the $N=4$ curve. Ultimately, when an infinite Hilbert space is used, the results for the g.s. energy should show a complete independence of $\hbar\Omega$ (i.e., C_a defined above vanishes) and should converge to the exact result of -24.55 MeV [14]. This is indeed the trend we are seeing in the $0\hbar\Omega$, $2\hbar\Omega$ and $4\hbar\Omega$ calculations but there is still a considerable gap between the $4\hbar\Omega$ results and the converged, exact value. Crude extrapolation of the C_a values for $N=0$, 2 and 4 indicates that one may have to do an $8\hbar\Omega$ calculation in order to reduce C_a to less than 0.1, at which point a 10 MeV change in $\hbar\Omega$ will, on average, results in less than 1 MeV change in the ground-state energy.

4 Auxiliary single-particle potential

The discrepancy between the energies obtained in the shell-model calculations of the preceding section and the exact result obtained for the RSC potential is due to the fact that some effective three- and four-body forces are ignored in our calculations.

Since shell-model calculations with inclusion of many-body forces are rather involved [9], we would prefer to find a way to diminish the effect of these many-body terms. For that purpose we consider the lowest-order contribution to the three-body folded diagrams displayed in Fig.1b. The contribution of this effective three-body force to the binding energy within the $0\hbar\Omega$ model space is represented by the diagram displayed in Fig.1c. If we introduce an auxiliary s.p. potential for all active states of the model space according to the BHF choice

$$\epsilon_i^{\text{BHF}} = t_i + \sum_{J,T} \frac{(2J+1)(2T+1)}{2(2j_i+1)} \langle (i\,0s)|G^T(\omega = \epsilon_i + \epsilon_{0s})|(i\,0s)\rangle_{J,T} \,, \qquad (11)$$

the contribution of the three-body term of Fig.1c and many higher-order diagrams originating from folding would be canceled by corresponding diagrams with s.p. insertions. Therefore, in this section, we would like to discuss the influence of introducing this auxiliary potential on the binding energy calculated in a $0\hbar\Omega$ model space.

It should be noted that Eq.(11) defines an auxiliary potential for the states within the model space. For s.p. states outside the model space we assume pure kinetic energy. This means that the Bethe-Goldstone Eq.(1) has been solved with the kinetic energy $(h_i = t_i)$ for the s.p. spectrum of the s.p. states outside the model space. The resulting G matrix is denoted by G^T, as we already did in Eq.(11). When one comes to calculate the BHF s.p. energies as defined in Eq.(11), this new choice for the intermediate energy spectrum is preferred, since our previous choice involves an unspecified shift V_0 in the one-body potential, which makes it difficult to unambiguously relate the starting energy with the BHF s.p. energies in Eq.(11).

In order to appreciate the significant effects of using the auxiliary potential, which

we will soon discuss, we need to separate the influence of the new choice for the intermediate spectrum on the results. To this end, we first evaluate the binding energy of ^{4}He in the $0\hbar\Omega$ model space without assuming an auxiliary potential. This means that we first solve Eq.(7) with $h_i = t_i$ for the new G-matrix

$$\left[t_1 + t_2 + G^T(\omega = E_{J,T})\right] \phi_{J,T} = E_{J,T}\, \phi_{J,T} \;, \tag{12}$$

so as to determine the matrix elements

$$\langle 0s^2|v_{\text{eff}}^{(2)}|0s^2\rangle_{J,T} = \langle 0s^2|G^T(\omega = E_{J,T})|0s^2\rangle_{J,T} \;. \tag{13}$$

We then evaluate the energy according to Eq.(6) and add the Coulomb repulsion between the two protons. Results for this calculation without an auxiliary potential are displayed in Fig.4 (solid line – "Without aux. pot."). These results are essentially the same as those we obtained in the previous section (Fig.3), indicating that the results are rather insensitive to the choice of the intermediate energy spectrum in the Bethe-Goldstone equation. This is also consistent with an earlier study [16] in which the role of the single-particle potential was examined in some detail at the level of two-body effective-interaction calculations. Here we extend those results to the case of starting-energy-independent effective two-body interactions. This is important since, by eliminating the issue of whether the single-particle insertions on intermediate particle lines are responsible for overbinding, we are then forced to consider the effective many-body forces that are addressed in the present study.

We now consider the BHF choice for the s.p. potential. We again use the one-dimensional model space for simplicity. In analogy to Eq.(8), we now have

$$\left[2\epsilon_{0s}^{\text{BHF}} + \langle 0s^2|G^T(\omega = E_{J,T})|0s^2\rangle_{J,T}\right] \phi_{J,T} = E_{J,T}\, \phi_{J,T} \;, \tag{14}$$

which determines the matrix elements of $v_{\text{eff}}^{(2)}$ according to Eq.(13). Results for the binding energy of ^{4}He with this choice of the auxiliary potential are also displayed in Fig.4 by the solid line labeled "With BHF pot.". One observes that the use of the

BHF auxiliary potential, which has been introduced to measure the effects of terms like the three-body folded diagrams of Fig.1b, reduces the calculated binding energy drastically. Even the minimal value for the binding energy (E_{gs}=-17.9 MeV), which is obtained around $\hbar\Omega = 16$ MeV, is well above the "exact result" of Ref.[14].

For the sake of comparison, we also show in Fig.4 the results (dotted line) for the BHF approximation (restricting the s.p. wave functions to the HO wave functions for a given $\hbar\Omega$), which can be obtained by replacing $E_{J,T} \rightarrow 2\epsilon_{0s}^{\text{BHF}}$. This approximation would correspond to a $0\hbar\omega$ no-core calculation, assuming the BHF auxiliary potential but ignoring the effects of two-body folded diagrams. We see that the two-body folded diagrams yield a repulsion of about 2 MeV. Such a repulsive effect has also been observed in shell-model calculations within the sd shell [8].

5 Conclusions

Energy-independent effective two-body interactions $v_{\text{eff}}^{(2)}$ are determined to calculate the g.s. energy of ^{4}He in three no-core HO model spaces with $\hbar\Omega$ ranging from 10 to 28 MeV. The results overbind the g.s. of ^{4}He for all the three spaces and for all the $\hbar\Omega$ values that we have used. The amount of overbinding is largest in the $0\hbar\Omega$ space and decreases as we increase the size of the model space from $0\hbar\Omega$ to $2\hbar\Omega$ and to $4\hbar\Omega$. The dependence of the calculated g.s. energy on the value of $\hbar\Omega$ also becomes weaker as the size of the model space increases. However, even in the $4\hbar\Omega$ calculation, the lowest g.s. energy of -31.9 MeV, which we obtained with $v_{\text{eff}}^{(2)}$ at $\hbar\Omega$=16 MeV, still overbinds ^{4}He by 3.6 MeV when compared with the experimental binding energy and by 7.3 MeV when compared with the binding energy obtained in the GFMC approach [14].

This overbinding is caused by the fact that we are neglecting some effective many-body forces. Our results using a BHF auxiliary potential, which includes certain effective many-body-force terms, show significant effects on no-core shell-model cal-

culations, especially when the model space is small. More studies are required to find an optimal auxiliary potential, which minimizes the effects of such many-body forces.

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Figure captions

Fig.1   Contributions to the effective three-body force originating from the so-called Q-box (a) and folded diagrams (b). The diagram (c) represents the contribution of diagram(b) to the ground-state energy within a $0\hbar\Omega$ model space. The bare lines refer to s.p. states within the model space while the "railed" lines respresent s.p. states outside the model space.

Fig.2   The two-body matrix elements, $\langle 0s^2|G(\omega')|0s^2\rangle_{J,T}$ (solid lines) and $\langle 0s^2|v_{\text{eff}}^{(2)}|0s^2\rangle_{J,T}$ (dotted lines) for the $4\hbar\Omega$ model space with $\hbar\Omega$=16 MeV as a function of the starting energy ω'. Note that the TBMEs of $v_{\text{eff}}^{(2)}$ are independent of ω'.

Fig.3   The ground-state energy of ^{4}He obtained from $v_{\text{eff}}^{(2)}$ as a function of $\hbar\Omega$ and N, the size of the model space.

Fig.4   The g.s. energy of ^{4}He as a function of $\hbar\Omega$ obtained from the $0\hbar\Omega$ calculation. Results are represented for using kinetic energies (labeled: Without aux. pot.) or BHF s.p. energies (label: With BHF pot.) as an auxiliary potential. For a comparison the dashed line displays the energies obtained with the BHF approximation.